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6. AUTHOR(S) C. Bray

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Aeronautics and Astronautics Southamton S09 5NH UK AFOSR-TR- 90 0823

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13. ABSTRACT (Maximum 400 words) A new theoretical description of mean chemical reaction rates in premixed turbulent commustion is devised. The mean rate is described as the product of the number of flamelet crossings per unit time and the average chemical production per crossing. Chemical mechanisms of arbitrary complexity can be accommodated. A generalised description of turbulent transport is proposed for use in combustor flow field calculations. The experimental programme was not successful because of illness and staff changes.

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Although the Research Assistant learned to use these techniques and successfully reproduced some earlier published data, no new data of publishable quality was obtained. The reason for this failure was the long term illness and eventual resignation of the Research Assistant.

Experimental data obtained by these methods is described in earlier publications^(2, 3).

3. Theoretical Work

The objective of the theoretical programme was the exploration of theoretical models suitable for prediction of dump combustor flowfields. The starting point of this work was the model of premixed turbulent combustion developed by the Principal Investigator in collaboration with Professor P. A. Libby of University of California, San Diego and Professor J. B. Moss of Cranfield Institute of Technology^(1, 4).

Important progress was made in two areas during the period of the grant as described below.

3.1 Scales of Scalar Field

Central features of the model of premixed turbulent combustion^(1, 4) which forms the subject of this research are (i) the description of the thermochemistry in terms of a progress variable c which may be defined as a normalised product species concentration and (ii) consideration of a combustion regime in which the turbulent flame consists of thin moving interfaces at the boundaries between packets of unburned and fully burned gas. The combustion reactions then occur only within these interfaces. In this combustion regime the time average heat release rate is controlled by the length or time scales which determine the interface structure and its frequency of occurrence.

The instantaneous equation for the progress variable c is written⁽⁵⁾

$$\frac{\partial}{\partial t}(\rho c) + \frac{\partial}{\partial x_k}(\rho u_k c) = (\rho D)_m \frac{\partial^2 c}{\partial x_k^2} + w \quad (1)$$

where w is the chemical source term and subscript m represents a mean value. For statistically stationary conditions the mean of this equation at high Reynolds numbers where molecular transport may be neglected is

$$\frac{\partial}{\partial x_k}(\overline{\rho u_k c}) = \overline{w} \quad (2)$$

where \overline{w} is the time average of the source term w . Our objective is to derive an expression for \overline{w} .

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We write⁽⁵⁾

$$\bar{w}(\underline{x}) = w_F(\underline{x}) \nu(\underline{x}) \quad (3)$$

where $\nu(\underline{x})$ is the frequency at which flamelet interfaces cross location \underline{x} and

$$w_F = \left\langle \int_F w dt \right\rangle \quad (4)$$

is the chemical reaction occurring per crossing, where subscript F indicates integration through a flamelet interface and the triangular brackets denote a time average.

The analysis⁽⁵⁾ may be divided into three parts. In the first part it is noted that, if the flamelet interfaces are thin, $c(\underline{x}, t)$ at a fixed point \underline{x} is a square wave time series between $c = 0$ and $c = 1$. This is modelled as a random telegraph signal, leading to the result that its autocovariance is⁽⁵⁾

$$P_{11}(\underline{x}, \hat{\tau}) \equiv \langle c(\underline{x}, t) c(\underline{x}, t + \hat{\tau}) \rangle = \bar{c}(1 - \bar{c}) \exp \left[-\frac{\nu \hat{\tau}}{2\bar{c}(1 - \bar{c})} \right] + \bar{c}^2 \quad (5)$$

The crossing frequency ν is determined as

$$\nu = 2\bar{c}(1 - \bar{c}) / \hat{T} \quad (6)$$

where \hat{T} is an integral time scale:

$$T = \int_0^\infty \frac{P_{11} - \bar{c}^2}{\bar{c}(1 - \bar{c})} d\hat{\tau} \quad (7)$$

A second stage of the analysis⁽⁵⁾ is the formulation of a balance equation for \hat{T} . This is done by writing Equation (1) at a location \underline{x}_1 and time t_1 and multiplying it by c evaluated at location \underline{x}_2 and time t_2 . Averaging then leads to a general two-point two-time covariance balance equation. The equation is specialised to one point and two times when it becomes a balance equation for the quantity P_{11} defined in Equation (5). Closure assumptions are made and the equation is integrated in $\hat{\tau}$ to give the required balance equation for $\hat{T}(\underline{x})$. The balance equation shows that, with the modelling assumptions already introduced, \hat{T} is a constant.

Main features of the above analysis have been confirmed experimentally as reported in the original publication and since verified elsewhere^(6, 7).

The last part of the analysis is to model the chemical term w_F which appears in (3). This is represented⁽⁵⁾ as

$$w_F = \frac{\rho_r S_L}{\tilde{u} \cos \bar{\theta}} \quad (8)$$

where ρ_r is the density of unburned mixture, S_L is the laminar burning velocity of that mixture, \tilde{u} is the Favre mean flow velocity, and $\bar{\theta}$ is the average angle between \tilde{u} and the direction normal to a flamelet. More recently⁽⁶⁾, Equation (8) has been replaced by an expression, based on an ensemble of strained laminar flamelets, which permits detailed chemical kinetics to be included.

An analysis of scalar length scales in premixed turbulent flames has also been reported⁽⁹⁾.

The advantages of the models described here, in comparison with earlier models, are that steps in the analysis can be tested experimentally and that detailed chemical kinetics of arbitrary complexity can be incorporated⁽⁸⁾.

3.2 Generalised Model for Turbulent Transport Fluxes

The model considered here⁽⁴⁾ is what is known as a second order closure model in which a separate balance equation is formulated and solved for each second order covariance term such as a Reynolds stress component $\overline{\rho u_j'' u_k''}$ or a mass flux component $\overline{\rho u_j'' c''}$. It is necessary to go to this level of sophistication because the pressure gradient transport terms, which form a major focus of the work, appear here.

Previous work^(1, 4) concentrated on planar one-dimensional turbulent flames separating regions of uniform flow in unburned and fully burned gases. Thus problems of modelling nonuniform turbulent flowfields in these unburned and fully burned regions were avoided.

The work reported here⁽¹⁰⁾ proposes a general three dimensional set of second order closure equations. Unlike the equations used previously^(1, 4) this set goes over properly to second order equations in the constant density low Mach number flows upstream and downstream of the turbulent flame.

A feature of second order closure models is that third order covariance terms appear and must be represented in terms of second order quantities. In the present work this is facilitated by the introduction of conditional velocities and turbulence quantities in reactant and product packets.

Thus for example⁽¹⁷⁾

$$\overline{\rho u_1'' u_j'' c''} / \bar{\rho} = \tilde{c} (1 - \tilde{c}) \left[(1 - 2c)(\bar{u}_{1p} - \bar{u}_{1r}) (\bar{u}_{jp} - \bar{u}_{jr}) + \overline{u_1' u_{jp}'} - \overline{u_1' u_{jr}'} \right] \quad (9)$$

where the flamelet interfaces are thin. Here subscripts r and p refer to conditional quantities in reactants and products, respectively, so that for example $\bar{u}_{1p} = \bar{c} u_1$.

The model derived⁽¹⁰⁾ from these considerations is

$$\frac{\overline{\rho u_1'' u_j'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} = (1 - 2\tilde{c}) \frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} \frac{\overline{\rho u_j'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} + s_{1j} \frac{\overline{\rho u_1'' u_j''}}{\bar{\rho}} \quad (10)$$

$$\begin{aligned} \frac{\overline{\rho u_1'' u_j'' u_m''}}{\bar{\rho}} = & - H_{1jm} + \tilde{c} (1 - \tilde{c}) \left[(1 - 2c) \frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} \frac{\overline{\rho u_j'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} \frac{\overline{\rho u_m'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} \right. \\ & + s_{1j} \frac{\overline{\rho u_1'' u_j''}}{\bar{\rho}} \frac{\overline{\rho u_m'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} + s_{jm} \frac{\overline{\rho u_j'' u_m''}}{\bar{\rho}} \frac{\overline{\rho u_1'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} \\ & \left. + s_{im} \frac{\overline{\rho u_1'' u_m''}}{\bar{\rho}} \frac{\overline{\rho u_j'' c''}}{\bar{\rho} \tilde{c} (1 - \tilde{c})} \right] \quad (11) \end{aligned}$$

where

$$H_{1jm} = c_s \frac{\tilde{k}}{\tilde{c}} \frac{\overline{\rho u_k'' u_m''}}{\bar{\rho}} \frac{\partial}{\partial x_k} \left(\frac{\overline{\rho u_1'' u_j''}}{\bar{\rho}} \right)$$

$$s_{1j} = (1 - K_{1j1})c + (K_{1j0} - 1)(1 - \tilde{c})$$

and c_s , K_{1j0} and K_{1j1} are constants; \tilde{k} and \tilde{c} are the turbulence kinetic energy and dissipation function respectively.

Modelling of other terms in the second order balance equations has been discussed elsewhere⁽¹⁰⁾. The resulting set of modelled balance equations has been solved for a simple one dimensional flow⁽¹¹⁾ with satisfactory results.

4. Recommendations and Conclusions

A major objective of the research programme was to propose a theoretical model for premixed turbulent combustion which would be suitable for use in dump combustor flowfields. Processes of transport⁽¹⁾ and turbulence production⁽⁴⁾ due to pressure gradients were to be taken into account. This objective has been met. The transport model recommended⁽¹⁰⁾ is that described above in Section 3.2. The turbulent chemistry model should be that outlined in Section 3.1 as modified in a recent publication⁽⁸⁾. The modification permits the inclusion of detailed chemical kinetic mechanisms of arbitrary complexity through the introduction of an ensemble of strained laminar flamelets.

The experimental objectives of the programme were not achieved. This was a severe disappointment and the need for such experiments remains although some of the gaps in the experimental picture have since been filled, for example in Refs. (6, 7, 12, 13).

Notation

c	progress variable
C_q	constant, see Eq. (11)
D	diffusion coefficient
E_{ij}	see Eq. (10)
H_{ijm}	see Eq. (11)
\tilde{k}	Favre mean turbulence kinetic energy
K_{ijo}	constant, see Eq. (10)
K_{iji}	constant, see Eq. (10)
P_{11}	autocovariance, see Eq. (5)
t	time
S_L	laminar burning velocity
\hat{T}	integral time scale, see Eq. (7)
u_i	i-th velocity component
w	chemical source term in Eq. (1)
w_F	see Eq. (3)
x_k	spatial coordinate
$\tilde{\epsilon}$	Favre mean viscous dissipation
$\bar{\theta}$	mean flame angle, see Eq. (8)
ν	flamelet crossing frequency
ρ	density
$\tilde{\tau}$	time delay

Subscripts

i, j, k, m	spatial coordinates
p	products
r	reactants

Other

$(\bar{\quad})$	mean value
$(\tilde{\quad})$	Favre mean value
$(\quad)''$	Favre fluctuation

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